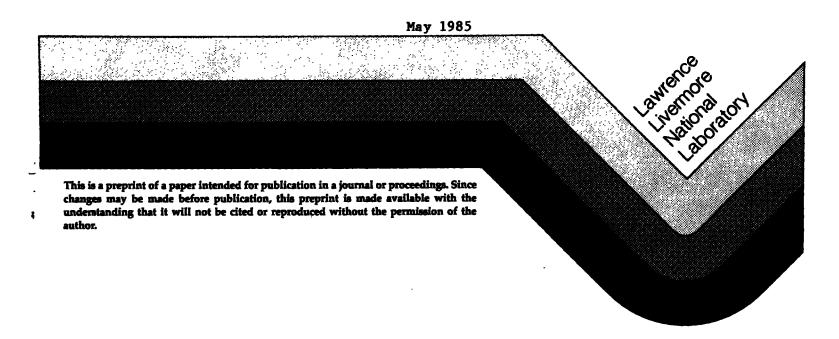
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LARGE-BASIS SHELL-MODEL TECHNOLOGY IN NUCLEOSYNTHESIS AND COSMOLOGY

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ABSTRACT We discuss various applications of the Lanczos method to describe properties of many-body microscopic systems in nucleosynthesis and cosmology. These calculations include: solar neutrino detectors; beta-decay of excited nuclear states; electron-capture rates during a core-bounce supernova; exotic quarked nuclei as a catalyst for hydrogen burning; and the quark-hadron phase transition during the early universe.

1. INTRODUCTION.

Often in astrophysics one is faced, at a computational level, with a need to know the eigenstates of a microscopic many-body system. Most often this appears as a need to know properties of unstable or unknown nuclear states. Similar needs can occur, however, for atomic states (e.g. opacities) or even high-temperature properties of the vacuum during the early universe. In this paper we briefly overview one particular technology (the Lanczos method) which has evolved in recent years as a means to calculate such non-relativistic Schrödinger-equation problems. We discuss the application of this algorithm to several current problems in nucleosynthesis and cosmology including; 1) The response of the $^{71}\text{Ga}(\nu,e^-)^{71}\text{Ge}$ solar-neutrino detector; 2) Beta decay rates for excited nuclear states; 3) The dynamics of neutronization during core-bounce supernovae; 4) The possibility of quarked nuclei as a catalyst for the p-p chain; and 5) The quark-hadron phase transition during the early universe.

2. THE LANCZOS METHOD

The Lanczos method (Whitehead, et al. 1977; Hausman 1976) is an iterative scheme to generate eigenstates and eigenvalues of a large basis without having to store the entire Hamiltonian matrix or even compute the entire spectrum of eigenstates. The procedure begins from an initial vector, |v₁>. Next, a new vector, orthogonal to the first, is constructed;

$$|v_2\rangle = [H|v_1\rangle - h_{11}|v_1\rangle]/h_{12}$$
, (1)

where $h_{ij} = \langle v_i | H | v_j \rangle$. This vector is then normalized and a third vector can be similarly constructed,

$$|v_3\rangle = [H|v_2\rangle - h_{21}|v_1\rangle - h_{22}|v_2\rangle]/h_{23}$$
.

This algorithm can be rearranged as a matrix equation,

$$H \begin{pmatrix} v_1 \\ v_2 \\ v_3 \\ \vdots \end{pmatrix} - \begin{pmatrix} h_{11} & h_{12} \\ h_{12} & h_{22} & h_{23} \\ & & h_{23} & h_{33} \\ & & & \ddots \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ v_3 \\ \vdots \end{pmatrix}$$
(3)

By diagonalizing this tridiagonal matrix after n iterations, one obtains n approximate eigenstates for the system. When n equals the dimension of the system this approach is an exact diagonalization. The power of this technique comes in, however, from the fact that the extrema of the spectrum converge first. Thus, if one is only interested in detailed properties for low-lying states and (or) average properties for high-lying states, adequate information can be obtained after a few Lanczos operations and the size of the matrix to diagonalize is miniscule.

This is the technique which we exploit. We are able to accommodate very large bases by using what we call the internal occupation-number representation, whereby the physical bits in the computer become the second-quantized occupation numbers. Thus, high-speed machine-language operations such as logical "or" and logical "and" become equivalent to the second-quantization creation and annihilation operators. This gives the code great speed and flexibility.

3. THE 71Ga(v,e-) 71Ge SOLAR NEUTRINO DETECTOR

As a first example, we consider the response of the proposed ⁷¹Ga neutrino detector. The ⁷¹Ga(v,e⁻)⁷¹Ge reaction has been much discussed as an experimental way to resolve the solar neutrino problem. The main nuclear physics reason that ⁷¹Ga is a good solar-neutrino detector is that the capture reaction has a low Q-value for the allowed ground-state to ground-state transition (about 233 keV). This low Q-value implies (Bahcall 1978) that a ⁷¹Ga detector should be sensitive mostly to neutrinos from the primary p+p+d+v+e⁺ reaction. The existing ³⁷Cl detector (Davis 1978), on the other hand, involves a bigger Q-value (814 keV) and is not sensitive to p-p neutrinos. The chlorine experiment is sensitive mainly to neutrinos from the decay of ⁸B.

Recently, there has been considerable discussion (Bahcall 1978; 1984; Orihara et al. 1983; Baltz et al. 1984; Grotz et al. 1984) concerning the contributions from neutrino captures which lead to excited states in ⁷¹Ge (see Fig. 1). In order to use ⁷¹Ga as a solar neutrino detector, one must know the cross sections for neutrino captures to excited states in ⁷¹Ge or show that they are unimportant. The larger Q-values for excited state transitions imply that these states are predominantly populated by neutrinos from the decay of ⁷Be and ⁸B.

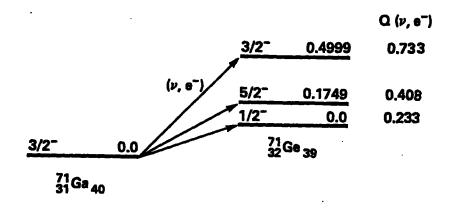


Figure 1 Transitions of interest for the $^{71}Ga(v,e^{-})^{71}Ge$ neutrino detector.

Our calculated (Mathews et al. 1985) GT strength to excited states in ⁷¹Ge is lower than the value inferred by Orihara et al. (1983) from the low-energy (p,n) data. Thus, our results support the analysis of Baltz et al. (1984) which indicates that the inferred £ = 0, zero-degree Gamow-Teller strength is overestimated in the 35 MeV experiment because of contributions from higher £-waves. Our results for the total neutron capture rate to the low lying levels in ⁷¹Ge, which are most important for solar neutrino experiments, (Bahcall 1978) are in generally good agreement with the previous

phenomelogical estimates (see Table 1). For the dominant sources, p-p and ⁷Be neutrinos, the total cross sections are practically identical when they are calculated with the nuclear model and with the phenomenological estimate. We do, however, calculate a somewhat larger capture rate to the lowest 5/2" state of ⁷¹Ge than was inferred from the beta-decay systematics and a somewhat smaller rate to the lowest 3/2" excited state. In addition, our nuclear model calculations suggest that there may be a large increase in the capture rate for ⁸B neutrinos (see Table 1) that is caused by Gamow-Teller (GT) transitions to excited states with energies between 2-6 MeV above the ground state of ⁷¹Ge.

Table 1. Calculated (Mathews et al. 1985) solar-neutrino capture rates (in SNU) compared with previous estimates.

Neutrino Source	Standard Solar Model Excited State Cross Sections:		Low Z Solar Model Excited State Cross Sections:		Mixed Solar Model Excited State Cross Sections:	
		(1978)		(1978)		(1978)
	p-p	70.2	70.2	72.5	72.5	74.2
pep	3.0	3.6	3.2	3.9	3.2	3.9
7 Be	31.2	31.7	10.9	11.1	11.2	11.4
⁸ в	11.6	1.2	1.6	0.3	2.4	0.4
13 _N	3.3	3.1	0.1	0.1	0.6	0.6
¹⁵ 0	4.6	4.7	0.0	0.1	1.0	1.0
[otal	124	115	88	88	93	92

4. BETA DECAY OF THERMALLY EXCITED NUCLEAR STATES

Thermally populated nuclear excited states occur in most realistic scenarios for neutron-capture nucleosynthesis (Mathews and Ward 1985). This thermal population of nuclear excited states can lead to drastically different beta-decay rates which affect the nucleosynthesis.

For example, the terrestrial beta-decay half life of 99 Tc is long ($t_{1/2} \sim 2 \times 10^5$ y) due to the second-forbidden decay of the $^{9/2+}$ ground state to the $^{5/2+}$ ground state of 99 Ru. There are, however, excited states at 140 and 181 keV in 99 Tc which can have GT

allowed transitions to the ground and first excited state of 99 Ru. If typical GT-allowed log(ft) values are assumed (Cosner et al. 1984) for these excited states the half life of 99 Tc reduces to about 1 yr. at Tq = 0.35 (kT=30 keV).

To understand ⁹⁹Tc nucleosynthesis it is important to know its thermally-enhanced beta-decay rate. In Fig. 2 we show our calculations (Takahashi, Bloom, and Mathews 1985) of low-lying states in ⁹⁹Tc, ⁹⁹Ru and the neighboring isotonic pair, ⁹⁷Nb-⁹⁷Mo. The energies are difficult to reproduce since the low-lying states are undoubtedly intruder states pushed down by the effects of coupling the $\pi(\lg_9/2)^3$ configuration to collective excitations of the core. On the other hand, the GT transition strength is probably dominated by the one-body components of these states and is probably adequately described by the limited model space employed here. Our calculations indicate that the stellar lifetime for ⁹⁹Tc may be considerably longer than previous estimates based on systematics (Cosner et al. 1984; Takahashi and Yokoi 1984).

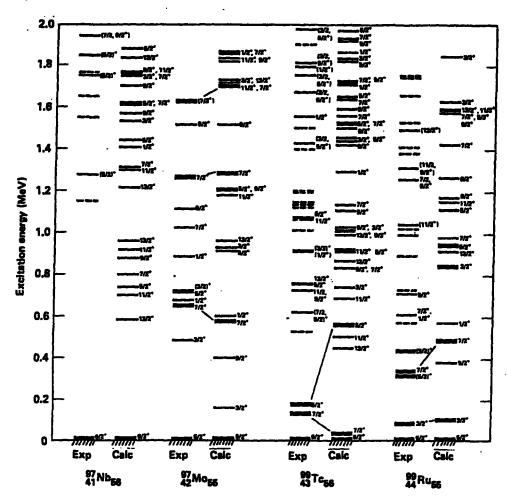


Fig. 2. Calculated (Takahashi et al. 1985) levels in ⁹⁹Tc, ⁹⁹Ru, and the neighboring isotonic pair, ⁹⁷Nb-⁹⁷Mo.

5. GAMOW-TELLER TRANSITIONS IN A PRESUPERNOVA STAR

Shell-model calculations of electron-capture transitions in iron-group nuclei are particularly important for determining the structure of presupernova massive stars. This structure then, in turn, determines whether a core-bounce supernova mechanism can occur. The role of the GT resonance in presupernova electron capture rates and the physics of stellar collapse have been described by a number of authors (Arnett 1977; Bethe et al. 1979; Weaver et al 1984; Fuller 1982; Burrows and Lattimer 1983).

A presupernova $\sim 25 M_{\odot}$ star (Woosley and Weaver 1982) at the end of silicon burning contains about a solar-mass of $^{54}{\rm Fe}$ and neutron-rich isotopes such as $^{48}{\rm Ca}$, $^{50}{\rm Ti}$, $^{54}{\rm Cr}$ and $^{58}{\rm Fe}$. As the core grows in mass it eventually becomes unstable to collapse when it reaches the Chandrasekhar mass (M $\sim 5.8 ({\rm Y_e})^2$), where ${\rm Y_e}$ is the ratio of free electrons to baryons). Electron capture rates will have an important effect in determining ${\rm Y_e}$ and therefore the Chandrasekhar mass.

Figure 3 is an example from some recent calculations (Bloom and Fuller 1984) of electron-capture GT strength for iron-group nuclei. This figure shows a calculation of the 56 Fe strength calculated in a two-particle two-hole configuration space for both the ground state and the $^{2+}$ first excited state. The GT resonance lies fairly low in energy, $^{32-5}$ MeV, and will participate in the neutronization. This resonance will speed the electron capture rate, and therefore reduce 32 Pe and the size of the Chandrasekhar mass relative to a calculation which has not included this resonance strength.

This is an important result since it makes the core-bounce mechanism more viable. The reason for this is that the core-bounce is actually experienced by an inner homologous (ver) core which then must photodisintegrate the outer core before impinging on outer envelopes of the star. To prevent the complete dissipation of the shock due to photodisintegration, the size of the outer core must be as small as possible, and the size of the inner homologous core must be large. The GT strength function (and the amount of GT quenching) will be important in determining both of these parameters. The total core mass will be small because the presupernova electron-capture rates are fast. On the other hand, the inner homologous core will be large due to the fact that the neutronization process will lead to Pauli blocking of the GT transitions as the core collapses. Thus, the inner homologous core does not benefit from the rapid electron capture rates which minimized the Chandrasekhar mass.

6. QUARKED NUCLEI IN THE SUN

Recently (Boyd et al. 1983) it has been suggested that free quarks (if present in an abundance of 10^{-15} and bound to nuclei) could act as a catalyst to the p-p chain in the sun. They would do this by making A = 5 nuclei stable and thus vastly decreasing the time it takes to build up to the $^{7}\text{LiQ}(p,\alpha)^{4}\text{He}$ reaction which completes the

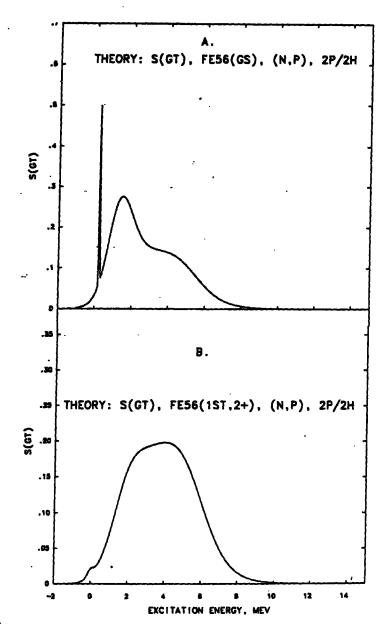


Fig. 3. Calculated (Bloom and Fuller 1984) GT strength for electron capture from the ⁵⁶Fe ground and first-excited state.

cycle. This hypothesis is contingent, however, on several assumptions. These are that ${}^5\!\mathrm{HeQ}$ is stable, that ${}^7\!\mathrm{BeQ}$ is unstable to electron capture, and that the ${}^7\!\mathrm{LiQ}(p,\alpha){}^4\!\mathrm{HeQ}$ reaction is energetically favored.

We were skeptical of these conditions and have attempted (Hughes et al. 1984) to at least qualitatively test them by calculating binding energies for quarked nuclei as best we could. We begin with a nuclear two-body force (Stone, et al. 1983) which reproduces the correct binding energies and charge radii for nuclei in this mass

range. The quark nucleon potential is expected to behave as a one-pion-exchange potential at large distances, so we use this interaction.

To our surprise we found that the necessary conditions for the quarked-nucleus p-p cycle could be obtained with "reasonable" values of a bare quark mass which is 4 times the nucleon mass and a potential strength which is 3 times the nucleon one-pion-exchange potential. We do not claim that this proves the validity of the quarked-nucleus hypothesis, but it does appear that we have been unable to disprove it.

7. THE QUARK-HADRON PHASE TRANSITION

At t $\sim 10^{-5}$ sec, T ~ 100 MeV, the universe is expected to have undergone a phase transition from a quark-gluon plasma to hadrons (mostly mesons). It has been speculated (Crawford and Schramm 1982) that this transition may introduce long-range fluctuations which could produce primordial black holes to act as seeds for galaxy formation. To date, however, this transition has not been studied in sufficient detail because of the complexity of the QCD vacuum although many efforts are underway. The most promising approach to understanding this problem is via a discretization of space-time on a lattice (lattice guage theory).

At a computational level the problem in lattice gauge theory is very similar to the many-body nuclear shell-model problem. We have already applied our code to solve for the phases of simple Z₂ and O(3) lattice guage theories. We are now in the process of upgrading the architecture of the code to accommodate the more challenging SU(3) QCD problem.

8. CONCLUSION

In this brief overview we have attampted to indicate a sampling of some of the kinds of problems in astrophysics which demand a solution to a non-relativistic quantum-mechanical many-body system. Some of the problems are difficult, but perhaps not impossible with technology currently available.

9. ACKNOWLEDGEMENT

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